

Energy Calculations of The Realistic Quantum Slab

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Abstract. We calculated the total energy of a semiconductor quantum dot which is defined by the trench gate method. In our calculation we used a recently developed energy functional called “orbital-free energy functional”. We compared the total energies obtained by Thomas-Fermi approximation, orbital-free energy functional and standard local-density approximation for the square quantum slab geometry. We have seen that this newly developed energy functional is numerically very efficient, superior to the Thomas-Fermi approximation and is in good agreement with the local-density approximation for two different sizes of quantum dot systems.

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1. Introduction

Applications of the two-dimensional (2D) quantum dots (QDs) and the rectangular quantum slabs (QSS) constitutes basic components of nanoelectronics and nanotechnology. Especially, the 2D electronic systems have attracted concern since the beginning of the developments in nanoelectronics and nanotechnology [1]. One of the most important problems in physics is handling of the electron-electron interactions concerning many-body systems. The Density Functional Theory (DFT) [2] offers a solution to the problem with a good accuracy with a reasonable computational cost. Furthermore, the DFT with two dimensional-local density approximation has become a standard method for the electronic structure calculations of the semiconductor QDs [3].

The most critical point of DFT is to describe the exchange and the correlation functionals in many-body systems[4]. Therefore new investigations in describing exchange and correlations of 2D density by functionals are important and lead to remarkable results [5, 6, 7, 8]. The local-density approximation (LDA) provides reasonably good results for the many-body systems, where the total density is the sole input variable instead of electronic orbitals as in the DFT. However, the number of electrons treated numerically is limited, since the Kohn-Sham (KS) scheme in DFT requires the computation of single particle KS orbital for the kinetic energy calculation [9]. An alternative theory, called orbital-free DFT [10, 11, 12] is more convenient than the traditional DFT. In contrast, this approach is more complicated in constructing an accurate energy functional especially for the three dimensional (3D) systems. An important example of orbital-free DFT is the traditional Thomas-Fermi approximation (TFA) that is analyzed in 2D [13] and is applied successfully in calculations of electronic structures [14]. However, the TFA treats the electron-electron (e-e) interaction only classically. Thus it is not a good approximation for small electron densities, *i.e.* in the strong interaction regime.

In this study, we use an orbital-free energy functional (OFEF) [9] to calculate the total energy of interacting electrons in two dimensions for different number of particle systems considering the QDs. In Ref. [9], the authors report quite consistent results with the local-density approximation and provide considerable improvements over the TFA. They also report that utilizing the orbital-free functional for 2DES is numerically very efficient by the virtue of orbital free calculation scheme and due to the calculation of Hartree integral.

In our study we calculate the energies of a quantum dot defined in quantum slab geometry, by using OFEF, TFA and LDA. These quantum dots are obtained by trench-gating [15].

2. Model

The realistic modeling of two-dimensional systems (2DES) relies on solving the 3D Poisson equation for given boundary conditions, set by the GaAs/AlGaAs

heterostructure and surface patterns, as shown in Fig.1-(a). The heterostructure consists of metallic surface gates determining the charge and the potential distributions, the 2DES, and δ -doped Silicon layer which provides electrons to the 2DES. The electron gas is formed at the interface of the GaAs/AlGaAs hetero-junction. The number of electrons, N and the average electron density, n_{el} are determined by the donor density n_0 and the metallic gates. To obtain the potential and the charge distribution of the system, first, the gate voltage V_g and the donor density are fixed and next the Poisson equation is solved self-consistently. For the solution, we used the code which based on a fourth-order algorithm operating on a square grid. This code is suitable for different boundary conditions which is applied and tested in previous studies [16, 17]. As an illustrating example in Fig. 1, the semiconductor surface is partially covered by a patterned gate or trench gate. Negatively charged metallic gate is biased with -1.0 V depicted by the black area as shown in Fig. 1-b. We used two different samples, namely Sample-I and Sample-II, with different slab's area corresponding to different density parameters r_s . The dimensions of the square slabs are $1.73\mu\text{m}$ and $1.11\mu\text{m}$ considering Sample-I and Sample-II, respectively. The bare confinement potential of the system can also be obtained analytically [15, 18], starting from the lithographically defined pattern. The un-patterned surface is taken to be pinned to the mid-gap of the heterostructure and is set to be the reference potential, $V_{unpat}(\mathbf{r}, 0) = 0$. The external potential $V_{ext}(x, y, z)$ is calculated for $z = 0$ plane by the solution of Laplace equation $\nabla^2 V_{ext}(\mathbf{r}) = 0$ and next we seek for a solution to the Poisson equation $\nabla^2 V_{ext}(\mathbf{r}) = 4\pi\rho(\mathbf{r})$, where $\rho(\mathbf{r})$ is the total charge density, considering the boundary condition $\partial V_{ext}/\partial z - > 0$ as $z - > \infty$.

3. Numerical Procedure and Results

In our numerical simulations we consider a unit cell containing the quantum dot which has the physical dimensions, $L_x = L_y = 7.9\mu\text{m}$ by a matrix of 128×128 mesh points. As an example, in Figs. 2 and 3, we show the charge distribution and the external potential profile only for $N = 20$ particles in the QS. Total energies of the Qs are calculated by using the potential and charge distributions obtained via solving the Poisson equation, self-consistently. The density parameter r_s can be used to define the average electron density in the quantum dot and this parameter is determined from $r_s = \sqrt{A/\pi N}$ considering hard wall boundary conditions for the quantum slabs, where A is the 2DES's area. In the standard TF approximation the total energy is given by

$$E[\rho] = T_{TF}[\rho] + \frac{1}{2} \int d\vec{r} \int d\vec{r}' \frac{\rho(\vec{r})\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} + \int d\vec{r} \rho(\vec{r}) v_{ext}(\vec{r}). \quad (1)$$

Since the electron-electron interactions are taken into account only classically, there is an important deficiency in Thomas-Fermi energy functional. Therefore in limited particle and low density regime, performance of this method is questionable due to the lack of the quantum mechanical effects such as exchange and correlation [9]. In order to improve TF approximation, a nonempirical, orbital-free energy functional for the

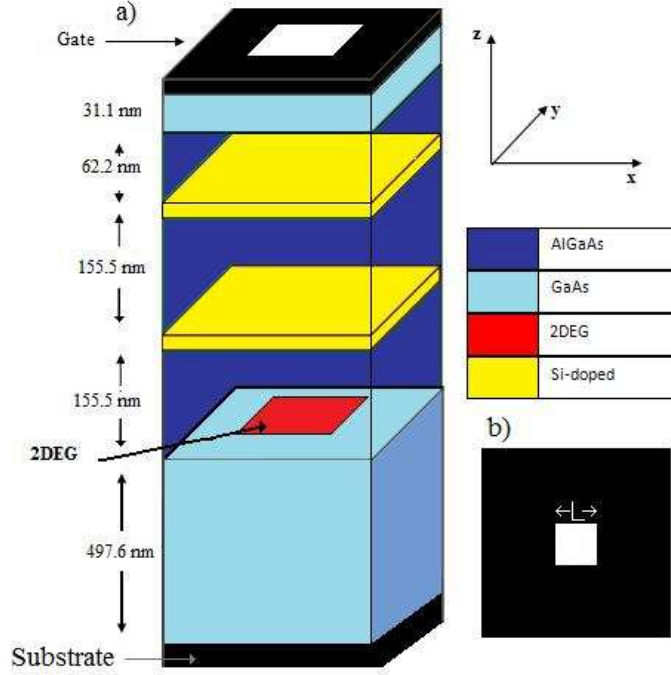


Figure 1. (a) The silicon doped heterostructure, the 2DES is formed at the interface of the GaAs/AlGaAs denoted by red region. The metallic gates are deposited on the surface. (b) Top view of the gate model of quantum slab, the edge width (L) of the square dot Sample-I and Sample-II are $1.73 \mu m$ and $1.11 \mu m$, respectively.

total energy of interacting electrons is proposed [9]. This functional is defined for the two-dimensional system as

$$E[\rho] = T_{TF}[\rho] + \frac{\pi}{2} \sqrt{\frac{N-1}{2}} \int d\vec{r} \rho^{3/2}(\vec{r}) + \int d\vec{r} \rho(\vec{r}) v_{ext}(\vec{r}). \quad (2)$$

It allows us to compute the total e-e interaction in a very simple form. We calculate and compare the total energies of Qs within orbital-free energy functional, Thomas-Fermi method and LDA.

In Fig. 4, we show the relative error in the total energy calculated within OFEF and LDA for QS considering various particle numbers. In Table I and II, the energies obtained from TF, OFEF and LDA are shown. By using the density and the potential profiles obtained from self-consistent procedure, we calculate the total energy of electrons in QS. In this work, we use the LDA energies obtained from OCTOPUS real-space DFT code [19] as the reference data. External confinement potential is obtained by a numerical interpolation utilizing a forth order polynomial fitting to the self-consistent potential.

From Table I, it is seen that the energy differences are not remarkably high for the QS up to $N = 60$ particles, while the differences are increasing for more number of particles. Meanwhile, our calculations show that the corresponding energy differences

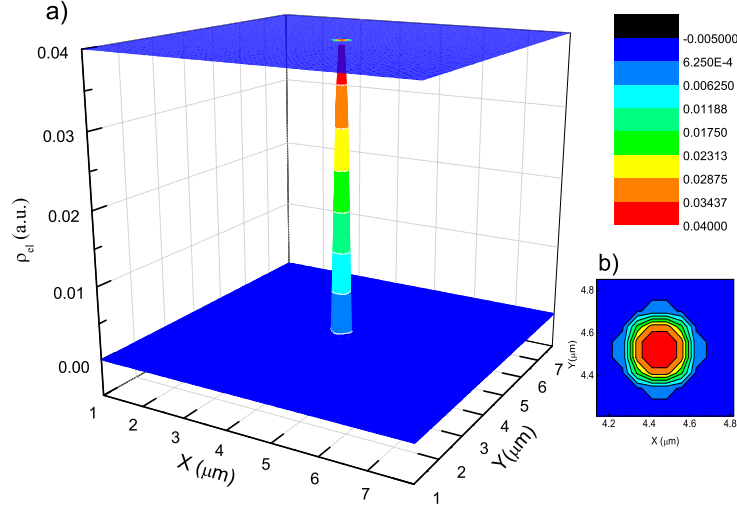


Figure 2. (a) Charge distribution of 2DES with square gate model for the quantum slab, the particle number N in the quantum dot is 20, Sample-II. (b) The top view of the charge distribution.

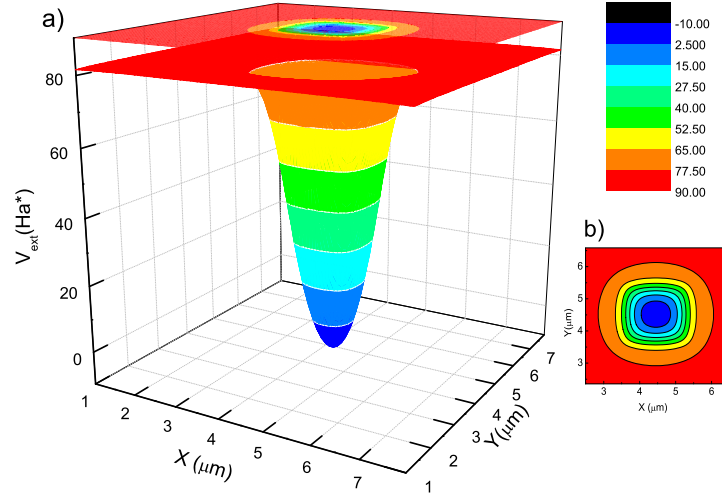


Figure 3. (a) Potential profile of 2DES with square gate model for the quantum slab, $N = 20$, Sample-II (b) top view of potential profile.

considering $N > 60$ particles are also affected by the density parameter r_s . We find a good agreement in the total energies between LDA and OFEF. Despite the TF results are also close to the reference data, the relative errors of orbital-free functional remains below the TF.

N	r_s	$-E_{OFEF}$	$-E_{TF}$	$-E_{LDA}$	$\Delta(\%)$
12	4.10	56.12	55.41	59.99	1.3
20	3.89	102.92	101.28	109.25	1.6
40	3.18	237.08	231.62	248.38	2.3
60	3.04	401.70	391.35	412.92	2.6
120	2.51	991.11	962.05	986.32	2.9
150	2.39	1369.80	1331.40	1353.70	2.8
200	2.36	2001.10	1940.50	1917.38	3.0

Table 1. Comparison of the total energy E values (in effective Hartree units) calculated within OFEF, TF approximation and LDA for Sample-I. The QS is defined by trench-gating. The last column defines relative errors, $\Delta = |(E_{TF} - E_{OFEF})/E_{OFEF}|$, considering N particles.

N	r_s	$-E_{OFEF}$	$-E_{TF}$	$-E_{LDA}$	$\Delta(\%)$
12	3.54	87.05	86.25	104.93	0.9
20	2.75	153.83	151.86	187.09	1.3
40	2.24	363.15	356.59	432.51	1.8
60	2.24	605.81	592.04	713.45	2.3
120	1.83	1488.1	1444.8	1715.66	2.9
150	1.74	2031.5	1973.20	2322.85	2.9
200	1.81	3012.90	2917.80	3383.74	3.2

Table 2. Comparison of the total energy E (in effective Hartree units) calculated within OFEF, TF approximation and LDA for Sample-II, similar to Table.1

4. Conclusion

In summary, we obtained the charge densities of QD systems by solving the 3D Poisson equation. Next, we utilized the obtained density considering a trench-gated structure to calculate the energy of the system by using the orbital-free functional, TF and LDA. According to our calculations, this new functional yields remarkably accurate results in many electron systems in the limit of low density and is very efficient due to its orbital-free form. Our future aim is to employ this calculation scheme to quantum point contacts and to investigate their transport properties.

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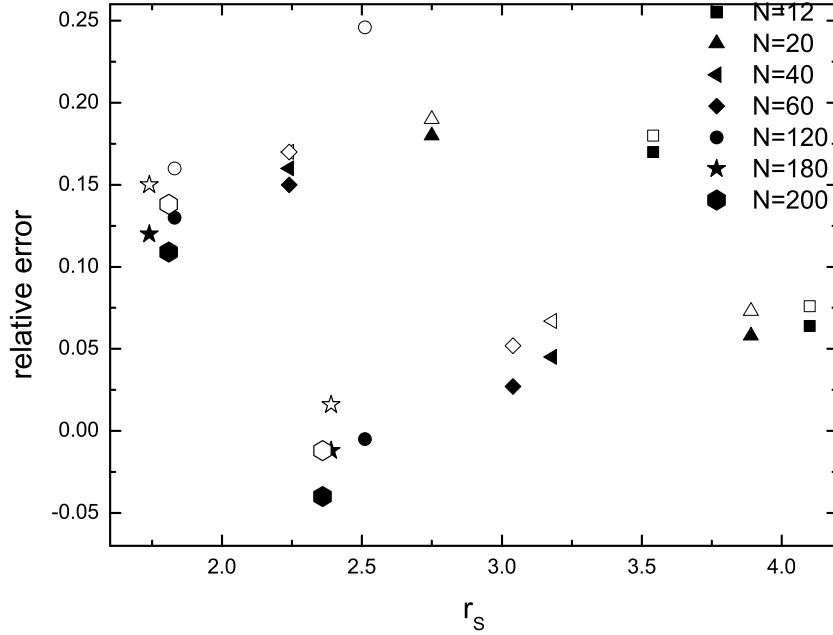


Figure 4. Relative error ($|E_{LDA} - E|/E_{LDA}$) in the total energy calculated within OFEF (filled symbols) and within the Thomas-Fermi approximation (open symbols) for rectangular quantum slabs with $N = 12, \dots, 200$ as a function of the density parameter r_s .

References

- [1] L. Jacak, P. Hawrylak, and A. Wójs, Quantum Dots (Springer, Berlin, 1998).
- [2] R.G. Parr and W. Yang. Density-functional Theory of Atoms and Molecules (Oxford University Press, New York/Clarendon, Oxford, 1989); R.M. Dreizler and E.K.U. Gross, Density functional theory (Springer, Berlin, 1990).
- [3] S. M. Reimann and M. Manninen, Rev. Mod. Phys. 74, 1283 (2002).
- [4] S. Sakiroglu and E. Räsänen, Phys. Rev. A 82, 012505 (2010)
- [5] E. Räsänen, S. Pittalis, C. R. Proetto, Phys. Rev. B 81, 195103 (2010)
- [6] S. Pittalis, E. Räsänen and C.R. Proetto, Phys. Rev. B 81, 115108 (2010)
- [7] P. Gori-Giorgi, M. Seidl and G. Vignale, Phys. Rev. Lett. 103, 166402 (2009)
- [8] L. A. Constantin, J. P. Perdew and J. M. Pitarke, Phys. Rev. Lett. 101, 016406 (2008)
- [9] S. Pittalis and E. Räsänen, Phys. Rev. B 80, 165112 (2009)
- [10] Y. A. Wang and E. A. Carter, in Theoretical Methods in Condensed Phase Chemistry, Progress in Theoretical Chemistry and Physics Series, edited by S.D. Schwartz (Kluwer, Dordrecht, 2000), pp. 117-184.
- [11] Ligneres V L and Carter E A, An Introduction to Orbital-Free Density Functional Theory (Springer, Netherlands, 2005)
- [12] S. C. Watson and E. A. Carter, Comput. Phys. Commun 128, 67 (2000)
- [13] E.H. Lieb, J.P. Solovej, and J. Yngvason, Phys. Rev. B 51, 10646 (1995).
- [14] A. Siddiki and R. R. Gerhadts, Phys. Rev. B 68 125315 (2003)
- [15] A. Siddiki and F. Marquardt, Phys. Rev. B 75, 045325 (2007).
- [16] S. Arslan, M.S. thesis, Technical University of Munich, 2008.

- [17] S. Arslan, E. Cicek, D. Eksi, S.Aktas, A.Weichselbaum and A.Siddiki, Phys. Rev. B 78, 125423 (2008).
- [18] J. H. Davies and I. A. Larkin, Phys. Rev. B 49, 4800 (1994).
- [19] A. Castro, H. Appel, M. Oliveira, C. A. Rozzi, X. Andrade, F. Lorenzen, M. A. L. Marques, E. K. U. Gross, and A. Rubio, Phys. Status Solidi 243, 2465 (2006) b.